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2-Amino-*N*-(2-methoxyphenyl)-4,5-dimethylthiophene-3-carboxamide

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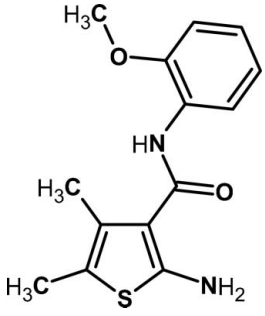
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.143; data-to-parameter ratio = 14.4.

In the title compound, $C_{14}H_{16}N_2O_2S$, the two aromatic rings make a dihedral angle of 13.9 (1)°. The crystal structure is stabilized by both inter- and intramolecular N—H···O, C—H···O and C—H···N hydrogen bonds.

Related literature

For related literature, see: Gewald *et al.* (1966); Cohen *et al.* (1977); Csaszar & Morvay (1983); Lakshmi *et al.* (1985); Mohan & Saravanan (2003); Bruns *et al.* (1990).



Experimental

Crystal data

$C_{14}H_{16}N_2O_2S$
M_r = 276.35
Monoclinic, $P2_1/n$
a = 8.606 (2) Å
b = 7.5193 (19) Å
c = 21.297 (5) Å
β = 100.599 (5)°
V = 1354.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 291 (2) K
0.45 × 0.35 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.908, T_{max} = 0.937
9834 measured reflections
2514 independent reflections
1503 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.142
S = 0.99
2514 reflections
175 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	2.15	2.724 (3)	124
N1—H1B···O1^{i}	0.86	2.23	3.009 (4)	151
N2—H2···O2	0.86	2.15	2.565 (3)	109
C8—H8···O1	0.93	2.30	2.874 (4)	119

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2721).

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supplementary materials

Figures

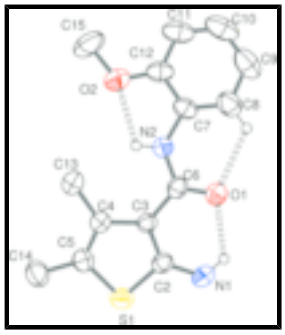

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.Dashed lines indicate intramolecular hydrogen bonds; H atoms not involved in hydrogen bonding have been omitted.

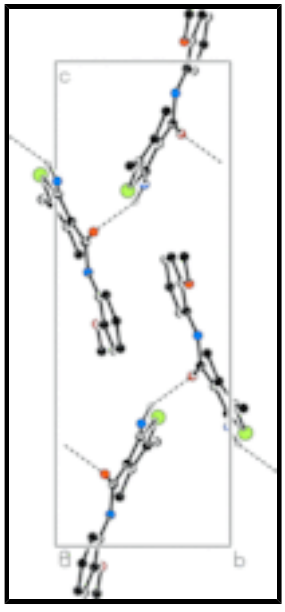

Fig. 2. The packing of (I), viewed down the *a* axis shows molecules connected by N—H···O hydrogen bonds (dashedlines). H atoms not involved in hydrogen bonding have been omitted.

2-Amino-N-(2-methoxyphenyl)-4,5-dimethylthiophene-3-carboxamide

Crystal data

$C_{14}H_{16}N_2O_2S$	F_{000} = 584
M_r = 276.35	D_x = 1.355 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2yn	Cell parameters from 670 reflections
a = 8.606 (2) Å	θ = 2.0–28.5º
b = 7.5193 (19) Å	μ = 0.24 mm^{-1}
c = 21.297 (5) Å	T = 291 (2) K
β = 100.599 (5)º	Block, yellow
V = 1354.7 (6) Å^3	0.45 × 0.35 × 0.28 mm
Z = 4	